Ozone Productivity of Atmospheric Organics

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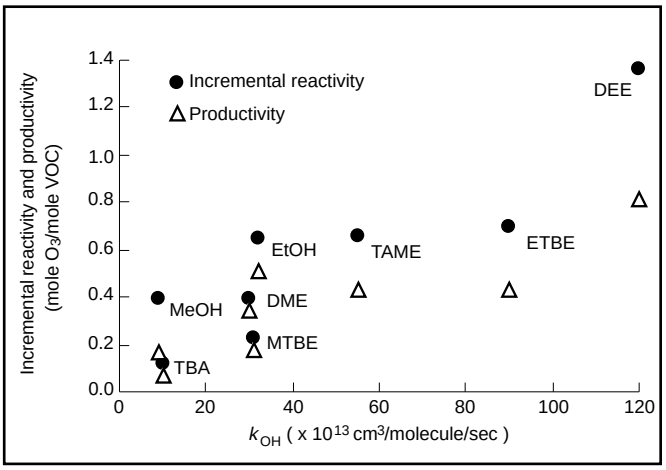
Objective

To determine the contributions to ozone (O_3) formation by individual volatile organic compounds (VOCs) in a complex VOC/oxides of nitrogen (NO_x) mixture and to examine the reactivity behavior of alternative fuels and reformulated gasoline (RFG) components.



Ozone production by fuel oxygenates

Approach

A method that assigns O_3 or other product species back to the original organic precursors is used to unravel the complex chemistry of a mechanism. These results are used to explain the incremental reactivity behavior of individual VOCs, including components of RFG and alternative fuels.

Accomplishments

The assignment method for determining individual VOC contributions to O_3 formation has been developed and used to analyze trajectory model results. These studies have shown that for an incremental reactivity calculation the overall change in O_3 is caused by changes in O_3 production by all species present, not only the incremented organic. The eight fuel oxygenates tested have relatively low incremental reactivities with values similar to those of alkanes and lower aromatics. This is due to their slow reaction rates, as well as the formation of relatively unreactive formate and acetate products. The fuel oxygenates that contain ethyl groups such as ethanol (EtOH) and ethyl tertiary butyl ether (ETBE) react faster and produce more ozone than those containing only methyl or tertiary butyl groups such as methanol (MeOH) and methyl tertiary butyl ether (MTBE).

Publications

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